Machine learning-based solution for thermo-mechanical analysis of MMIC packaging

Sumin Kang (suminkang@kimm.re.kr)
Korea Institute of Machinery & Materials (KIMM)

Jae Hak Lee
Korea Institute of Machinery & Materials (KIMM)

Seung Man Kim
Korea Institute of Machinery & Materials (KIMM)

Jaeseung Lim
Chonnam National University

Ah-Young Park
Korea Institute of Machinery & Materials (KIMM)

Seongheum Han
Korea Institute of Machinery & Materials (KIMM)

Jun-Yeob Song
Korea Institute of Machinery & Materials (KIMM)

Seong-Il Kim
Electronics and Telecommunications Research Institute

Article

Keywords:

Posted Date: August 8th, 2022

DOI: https://doi.org/10.21203/rs.3.rs-1931145/v1

License: This work is licensed under a Creative Commons Attribution 4.0 International License. Read Full License
Abstract

Thermo-mechanical analysis of monolithic microwave integrated circuit (MMIC) packaging is essential to guarantee the reliability of radio frequency/microwave applications. However, a method for fast and accurate analysis of MMIC packaging structures has not been developed. Here, we demonstrate a machine learning (ML)-based solution for thermo-mechanical analysis of MMIC packaging. This ML-based solution analyzes temperature and thermal stresses considering 13 design parameters categorized into material properties, geometric characteristics, and thermal boundary conditions. Finite element simulation with the Monte Carlo method is utilized to prepare 40,000 data samples for supervised learning and validation of the ML solution, and a laser-assisted thermal experiment verifies the accuracy of the simulation. After data preparation, regression tree ensemble and artificial neural network (ANN) learning models are investigated. The results indicate that the ANN models accurately predict the temperature and thermal stresses, showing a 1.69 % minimum error. Finally, the developed ML solution is deployed as a web application format for facile approaches. We believe that this study will provide a guideline for developing ML-based solutions in chip packaging design technology.

Introduction

Monolithic microwave integrated circuits (MMICs) have led to rapid advances in radio frequency (RF) applications, including 5G base stations, automotive radar, and satellite communication systems\(^1\)\(^-\)\(^4\). In this regard, a packaging strategy considering temperature and thermal stresses is key to ensuring the reliability of the MMICs because the large amount of heat generated by the high power density and small form factor often causes thermo-mechanical failure\(^5\)\(^-\)\(^9\). An MMIC packaging structure involves many design parameters, such as material selection for each part, geometric characteristics, and thermal boundary conditions (BCs). In this context, obtaining analytical or empirical solutions to analyze the MMIC packaging structure is a formidable task owing to the nonlinearly correlated and high-dimensional design parameters. Multiphysics finite element method (FEM) simulation can provide accurate prediction results for the MMIC packaging structure\(^10\)\(^-\)\(^13\). However, additional FEM simulations have to be conducted whenever the design parameters are changed, resulting in high computing costs and time-consuming processes. Therefore, a facile, fast, and accurate solution for thermo-mechanical analysis of the MMIC packaging problem is required.

A machine learning (ML) framework has recently been utilized to analyze various engineering problems, including cardiovascular organs\(^14\)\(^-\)\(^16\), cantilevered structures\(^17\),\(^18\), and composite materials\(^19\),\(^20\). In particular, the ML framework allows the prediction of critical reliability parameters in chip package structures, such as energy release rates\(^21\), warpage behaviors\(^22\), and drop responses\(^23\). Furthermore, several studies have presented analysis models for the accelerated reliability of solder joints under thermal cycling conditions using artificial neural network (ANN) architectures\(^24\)\(^-\)\(^26\). These ML approaches driven by FEM simulation data have been regarded as a fast and accurate surrogate of the simulation.
However, despite these successful efforts, an ML-based analysis for MMIC packaging concerns has not yet been developed.

In this study, we present an ML-based solution for thermo-mechanical analysis of MMIC packaging that determines the maximum values of temperature and thermal stresses of chip–adhesive–carrier–housing packaging structures considering 13 design parameters categorized into materials properties, geometric characteristics, and thermal BCs. FEM simulation with the Monte Carlo method was conducted to prepare training and test datasets, and a laser-assisted thermal experiment validated the simulation results. The prepared datasets were utilized for the supervised learning of regression tree ensemble and ANN models, and the minimum errors of each ML model were investigated by optimizing their hyperparameters. Finally, we deployed the developed ML solution as a web application format for facile approaches for general users.

Results And Discussion

Outline of the ML-based solution for the MMIC packaging problem. Figure 1 outlines the ML-based fast and accurate analysis solution for MMIC packaging structures. The ML solution was designed to provide thermo-mechanical analysis results when several design parameters were input into the ML model, which was constructed based on experimentally validated simulation data. In this regard, 13 design parameters related to material properties, layer thickness, and thermal BCs were defined considering the traditional gallium-nitride (GaN)-based MMIC packaging structure composed of chip–adhesive–carrier–housing. In the structure, 4H-silicon carbide (SiC) and Al6061 alloy were used as the chip and housing materials, respectively, because GaN transistors are typically produced on high-quality 4H-SiC chips, and the low density of Al6061 is advantageous for reducing weight. In contrast, many suitable candidates for the adhesive and carrier materials were available. Accordingly, the material properties of the adhesive and carrier (thermal conductivity, coefficient of thermal expansion (CTE), elastic modulus, and Poisson’s ratio) were regarded as the input variables. Moreover, the thicknesses of the chip, adhesive, and carrier layers were adjustable input variables, which can influence the heat transfer performance and thermal deformation behaviors. Finally, a surface heat flux was applied to a local region on the top surface of the chip, reflecting thermally dissipated power, and convection cooling was applied to the bottom surface of the housing. These thermal BCs (surface heat flux and heat transfer coefficient) were regarded as important variables in the MMIC packaging design.

The output analysis results were defined as the maximum values of temperature in the MMIC package structure, principal stress in the chip, and von Mises stress in the adhesive. These output variables are critical indicators for predicting failure behaviors of the MMICs. The MMIC devices require qualified operating and storage temperatures due to thermal degradation. Moreover, thermal stresses in the MMIC structure are caused by CTE mismatch and warpage behavior, often resulting in failures of the chip and adhesive parts. Despite the high fracture strength of 4H-SiC, the thermal stress in the chip causes chip cracking due to the presence of material defects such as micro-cracks, scratches on the
surface, and chipping on the edges\textsuperscript{35–37}. In addition, cracking or delamination behaviors in the adhesive are frequently caused by the stress concentration effect\textsuperscript{38,39}.

**FEM simulation for data preparation and its experimental validation.** After defining the input and output variables, FEM simulation was performed to prepare a large dataset for supervised learning. Figure 2a shows a 3D model of the chip–adhesive–carrier–housing MMIC packaging structure. In this model, 4H-SiC and Al6061 were assigned for the chip and housing, respectively, and the materials properties of the adhesive and carrier were changed based on various material candidates. The assigned material properties are represented in Table S1. The in-plane dimensions of the chip, adhesive, and carrier were fixed at $5 \times 5 \text{mm}^2$, $5 \times 5 \text{mm}^2$, and $11 \times 14 \text{mm}^2$, respectively, and the housing had a constant dimension of $50 \times 50 \times 10 \text{mm}^3$. The layer thicknesses varied in the ranges of $30–200 \mu\text{m}$, $10–100 \mu\text{m}$, and $0.3–2.5 \text{mm}$ for the chip ($x_9$), adhesive ($x_{10}$), and carrier ($x_{11}$), respectively. Furthermore, the surface heat flux ($x_{12}$) was changed in the range of $1–30 \text{W}$, and the heat transfer coefficient ($x_{13}$) was changed in the range of $0–300 \text{W/m}^2\cdot\text{K}$. Detailed information on the FEM simulation is described in the Methods section. Consequently, 40,000 samples of a dataset were prepared by randomly assigning input values within the defined ranges for each variable and obtaining the corresponding output values with the FEM simulation. The prepared dataset is presented in Table S2.

Figure 2b shows a 3D quarter simulation model of the MMIC packaging structure and its temperature distribution. The quarter model in the simulation was suitable owing to the x- and y-axis symmetry conditions, which significantly reduced the calculation time. The enlarged view in Fig. 2b indicates that the maximum temperature was located at the center of the heat source region, and the temperature decreased gradually as the distance from the center point increased (Figure S1). Figures 2c and 2d depict the distribution of thermal stresses in the chip and adhesive. The maximum principal stress, which is a representative failure criterion of brittle materials, was located inside the chip. The maximum von Mises stress was located at the edge of the adhesive, indicating the potential for interfacial delamination due to peeling moments\textsuperscript{40}.

To evaluate the accuracy of the simulation data, we conceived a laser-assisted thermal testing method (Fig. 3a). In the experiment, the center point of the top surface of the MMIC chip was irradiated for 15 min with a 532 nm continuous-wave laser beam with 2.5 W input power, and a thermal imaging camera measured the maximum temperature. MMIC packaging specimens which were composed of 4H-SiC chip–sintered Ag adhesive–carrier–Al 6061 housing structures, were tested with respect to two types of carrier materials, Ag diamond and CuW. The specimens were placed on an x–y–θ controllable alumina stage that acted as a heat spreader by dissipating accumulated thermal energy from the packaging structure. The experimental results for the two cases show that the maximum temperature values obtained in the simulation agreed well with the experiment, thereby verifying the accuracy of the simulation data (Fig. 3b). Furthermore, it was observed that the Ag diamond carrier, which has a high thermal conductivity of 700 W/m·K, enabled a reduction in the maximum temperature compared to that of the CuW carrier owing to the enhanced heat transfer performance\textsuperscript{30}.
Development of the ML-based solution. The prepared simulation dataset of 40,000 samples was divided into an 80% training dataset for supervised learning of the ML model and a 20% test dataset for evaluating the accuracy of the ML model. Furthermore, regression tree ensemble and ANN models were utilized to obtain an optimal ML model for the MMIC packaging analysis. The regression tree ensemble model is composed of a cluster of regression trees that provides more accurate results by synthesizing the responses from each tree (Fig. 4a). In particular, we focused on the two gradient boosting models, eXtreme Gradient Boosting (XGBoost) and Light Gradient Boosting Machine (LightGBM), which are regarded as scalable, flexible, and versatile tools owing to their regularization technique. The main difference between XGBoost and LightGBM is the growth strategies of each tree (Fig. 4b). The trees in XGBoost are grown by splitting all nodes on the same layer simultaneously. In contrast, the trees in LightGBM are grown by expanding nodes in best-first order instead of a fixed order, allowing high computational efficiency.

To investigate the optimum prediction performance of the regression tree ensemble models, two hyperparameters, the number of trees and maximum tree depth, were controlled. The number of combining trees in the ensemble models was set at 128, 256, and 512, and the tree depth (i.e., the maximum number of edges from the root node to the leaf node as shown in Fig. 4b) was controlled in the range of 6–12. Detailed information on the regression tree ensemble models is described in the Methods section. The evaluation index for the accuracy of the solution was determined as the mean absolute percentage error (MAPE) as follows:

\[
\text{MAPE} = \frac{100\%}{3} \sum_{i=1}^{3} \frac{y_i - \hat{y}_i}{y_i}
\]

where \(y_i\) is a true value of the simulation and \(\hat{y}_i\) is a predicted value obtained from the ML solution. In this context, five-fold cross-validation was adopted to enhance the reliability of the results.

Figures 4c and 4d show the results of the XGBoost and LightGBM models, respectively. It was found that the ensemble models with 512 trees predicted the results more accurately than those with the 128 and 256 ensemble trees, and there were optimum values of the tree depth in a moderate range due to overfitting. The minimum errors of the two models were similar: 5.34% for XGBoost and 5.21% for LightGBM. Meanwhile, owing to the efficient growth strategies, the training time of the LightGBM model was approximately six times faster than that of the XGBoost model. These results indicate that the LightGBM model is advantageous compared to the XGBoost model for the MMIC packaging analysis. However, the prediction accuracies of regression tree ensemble models were deemed insufficient to utilize as a surrogate of the simulation for the MMIC packaging problem, even though their training time was very fast.
Meanwhile, the ANN models, inspired by biological neural systems, have great potential for accurate prediction of outcomes considering complex nonlinearities in a dataset\textsuperscript{44,45}. The typical structure of fully connected ANN models comprises the input layer, hidden layers, and output layer (Fig. 5a). In this context, the number of nodes in the input and output layers was fixed at 13 and three, corresponding to the number of input and output variables, respectively. In contrast, the number of hidden layers and the number of nodes in each hidden layer are controllable and can significantly influence the prediction results. Therefore, we investigated the prediction accuracies of the ANN models by altering the number of hidden layers in the range of 1–7 and the number of nodes in the range of 16–512. The ANN structures were denoted as \( n_i/n_1/n_2/\ldots/n_k/n_o \), where \( n_i, n_1, n_2, n_k, \) and \( n_o \) are the number of nodes in the input layer, hidden layers, and output layer, respectively. Detailed information on the ANN models is described in the Methods section.

The 3D graph in Fig. 5b shows the errors of each ANN model. The shallow and narrow structure of 13/16/3 showed a high error of 14.93% due to the small number of perceptrons; however, the error gradually decreased as the number of hidden layers and nodes increased. The minimum error of 1.69% was observed in the 13/128/128/128/128/128/3 structured ANN model. Moreover, the error was slightly increased in more complex structures, indicating the possibility of overfitting. Based on these investigations, that the ANN models exhibited superior prediction performance compared with those of the regression tree ensemble models due to the high dimensionality of the dataset. The developed ML solution provides accurate analysis results within a few seconds, whereas conventional FEM simulation requires a few minutes to hours, depending on the mesh size. Finally, we deployed the optimal ANN model as a web application format which facilitates the use of the solution by a graphical user interface (Figure S2)\textsuperscript{46}. Moreover, users can refer to the source code of the web application in a public cloud to develop new solutions for other engineering problems.

**Conclusion**

We developed an ML solution for the thermo-mechanical analysis of MMIC packaging using experimentally validated FEM simulation data. The ML solution was designed to output the maximum values of temperature and thermal stresses considering several input parameters related to material properties, geometric characteristics, and thermal BCs. The FEM simulation dataset was used in the training and testing of the ML model, and a laser-assisted thermal experiment verified the accuracy of the simulation data. The prediction accuracies of regression tree ensemble and ANN models were evaluated by adjusting hyperparameters. The results showed the ANN model predicted the outcomes more accurately than the regression tree models due to the high dimensionality of the dataset. Finally, the ML solution based on the ANN model was shared as a web application to facilitate the use of the solution for researchers and engineers. The ML solution provides accurate thermo-mechanical analysis results with extremely low computing time and a simplified process. We believe that the presented method can contribute to advances in design technology by expanding to many engineering problems, not only the electronic packaging.
Methods

**FEM Simulation.** Commercial software (Abaqus 6.14-3) was used for the FEM simulation. The 3D-quarter model of the chip–adhesive–carrier–housing structure was created as a deformable solid using the x- and y-axis symmetric conditions. A tie constraint of the interfaces between adjacent layers was assigned. The dissipated heat and convection cooling were assigned as the surface heat flux and heat transfer coefficient, respectively, and the initial temperature was set at 25°C. In addition, natural convection cooling with a coefficient of 5 W/m²·K was assigned to the other exposed surfaces. Regarding the boundary conditions, the z-axis (out-of-plane) displacement of the bottom surface of the housing was constrained, and a center point at the surface was additionally constrained with an encastre to prevent rotation and translation of the model. After modeling, a rectangular-shaped mesh with a temperature–displacement coupled type (C3D8T, an 8-node thermally coupled brick, trilinear displacement and temperature) was applied.

**Regression tree ensemble models.** The XGBoost and LightGBM models were introduced using the open-source python packages. The learning rate and boosting type were set at 0.05 and gradient boosting tree, respectively. The upper bound of the tree depth was controlled in the range of 6–12, and the number of weak learners was controlled with 128, 256, and 512 trees. In particular, the number of leaves in the LightGBM model was defined as $2^{(\text{depth}-1)}$, considering the characteristics of the growth strategy. The MultiOutputRegressor package was utilized to simultaneously calculate three outputs in the XGBoost and LightGBM models.

**ANN models.** The ANN models were trained using the open-source platform TensorFlow. Fully connected ANN models with the ReLU activation function were generated, and the Adam optimizer, mean absolute error loss function, and 5000 epochs were adopted for training the ANN models. The number of hidden layers and the number of nodes in each layer were controlled as the hyperparameters, in the ranges of 1–7 layers and 16–512 nodes.

Declarations

**Acknowledgments**

This work was supported by the Convergence Research Center Program (CRC-19-02-ETRI) of the National Research Council of Science & Technology (NST) funded by the Ministry of Science and ICT (MSIT), the Technology Innovation Program (20014846), and the Industrial Strategic Technology Development Program (1415168490) of the Korea Evaluation Institute of Industrial Technology (KEIT) funded by the Ministry of Trade, Industry and Energy (MOTIE).

**Author contributions**

S.K. and J.H.L. conceived the idea of the project. S.K. performed data collection and analysis, and wrote the manuscript. J.L. supported the laser-assisted experiment under the guidance of S.M.K. All authors
discussed the results and reviewed the manuscript.

**Competing interests**

The authors declare no competing interests.

**Additional Information**

**Supplementary Information** The online version contains supplementary material available at –

**Correspondence** and request for materials should be addressed to S.K.

**Reprints and permissions information** is available at –

**Data availability**

The datasets generated and/or analyzed during the current study are available from the corresponding author on reasonable request.

**References**


**Figures**

**Figure 1**

ML-based solution for fast and accurate analysis of MMIC packaging.
Figure 2

Simulation modeling and representative results. (a) 3D full model of MMIC packaging structure. (b) 3D quarter model in the simulation and its temperature profile. (c) Principal stress distribution in the chip. (d) Von Mises stress distribution in the adhesive.

Figure 3

Experimental validation of the simulation results. (a) Experimental setup for measuring the maximum temperature of the MMIC packaging structure. (b) Maximum temperature of the MMIC packaging...
structures for two different carrier materials, Ag diamond and CuW.

Figure 4

Results of regression tree ensemble models. (a) Schematic of a regression tree ensemble structure composed of a set of weak regression trees. The ensemble structure predicts the results by aggregating responses from each regression tree. (b) Two different tree growth strategies denoted as level-wise tree growth for XGBoost and leaf-wise tree growth for LightGBM. Prediction results of the (c) XGBoost and (d) LightGBM models with respect to the number of trees and tree depth.
Figure 5

Results of ANN models. (a) Schematic of fully connected ANN structure composed of the input layer, hidden layers, and output layer. (b) The prediction results of ANN structures with respect to the number of hidden layers and nodes.

Supplementary Files

This is a list of supplementary files associated with this preprint. Click to download.

- SupplementaryInformationKang.pdf